

Bosons with attractive interactions in a trap: Is the ground state fragmented ?

Ø. Elgarøy^a and C. J. Pethick^b

^a*Department of Physics, University of Oslo, N-0316 Oslo, Norway*

^b*Nordita, Blegdamsvej 17, DK-2100 Copenhagen Ø, Denmark*

Possible fragmentation of a Bose-Einstein condensate with negative scattering length is investigated using a simple two-level model. Our results indicate that fragmentation does not take place for values of the coupling for which the system is metastable. We also comment on the possibility of realizing a fragmented condensate in trapping potentials other than an harmonic one.

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Bose-Einstein condensation in dilute atomic gases has been an area of intense activity since the first experimental realizations of these systems [1–3]. The experiments have so far been carried out with the alkali atoms ⁸⁷Rb, ²³Na, and ⁷Li. While the s-wave scattering length is positive in the first two cases, it is negative for ⁷Li, implying that the effective atom-atom interaction is attractive. A homogeneous system of these atoms will collapse to a dense state before densities where a Bose-Einstein condensate can form are reached [5]. However, in the experiments Bose condensation is realized under inhomogeneous conditions, and theoretical calculations show that the system may then be metastable as long as the number of condensed particles is below a critical value, $N_c \sim 10^3$ for ⁷Li [4,6] for the trap used in the experiments. The latest experiments are consistent with this result [7].

The homogeneous Bose gas with attractive interactions was considered in a paper by Nozières and Saint James [8]. While their main interest was the onset of a BCS-like transition, they also asked whether a fragmented Bose condensate would form. In the homogeneous case, fragmentation means that the particle distribution in momentum space, $n_{\mathbf{k}}$ has a sharp peak near $\mathbf{k} = 0$ which extends over a number of $(\mathbf{k}, -\mathbf{k})$ states large compared to 1, but small compared to the particle number N : on a macroscopic scale, it looks like a δ -function. That this is a reasonable question can be seen within the Hartree-Fock approximation: for bosons with an attractive interaction the Fock term makes it energetically favorable to spread the particles over several states. Still, the authors of Ref. [8] found that fragmentation of the condensate does not take place in a homogeneous system. However, the physics of the inhomogeneous Bose gas is different, and it seems worthwhile to ask the same question again in this context.

We want to study the ground state of bosons with a negative s-wave scattering length in an isotropic harmonic oscillator potential. Since the question we are addressing is whether the condensate can fragment, we must allow for (at least) two single-particle states in the calculation. We will consider the two normalized single-particle wave functions

$$\psi_0(\mathbf{r}) = \frac{1}{\pi^{3/4} b^{3/2}} e^{-r^2/2b^2} \quad (1)$$

$$\psi_1(\mathbf{r}) = \frac{2^{1/2}}{\pi^{3/4} b^{5/2}} z e^{-r^2/2b^2} \quad (2)$$

where $r^2 = x^2 + y^2 + z^2$ and b is a variational parameter. These have the same shape as the ground state and the first excited state with angular momentum projection $m_l = 0$ of the harmonic oscillator well. There will be interactions between particles in the different levels and also between particles in the same level. For fixed b the many-body Hamiltonian is

$$\hat{H} = \sum_i \langle i | \hat{t} + \hat{u} | i \rangle \hat{a}_i^\dagger \hat{a}_i + \frac{1}{2} \sum_{ijkl} V_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l \quad (3)$$

where $i, j, k, l = 0, 1$, \hat{t} is the kinetic energy operator, $\hat{u} = \frac{1}{2} m \omega^2 r^2$ and

$$V_{ijkl} = -\frac{4\pi\hbar^2|a|}{m} \int d^3r \psi_i^* \psi_j^* \psi_k \psi_l, \quad (4)$$

where a is the scattering length (assumed negative) and m is the boson mass. We will in the following solve this two-level problem for arbitrary values of b , thus obtaining the ground state energy of the model as a function of this variational parameter. In the next step b is determined by minimizing the energy. This simple two-level system can be solved exactly and is in fact a special case of the so-called Lipkin model [9] which has been widely used in nuclear physics as a tool for studying many-body approximation methods.

We now proceed by writing out the Hamiltonian in Eq. (3) in more detail. The single-particle matrix elements are given by

$$\langle 0 | \hat{t} + \hat{u} | 0 \rangle = \frac{3}{4} \hbar \omega \left(x^2 + \frac{1}{x^2} \right) \quad (5)$$

$$\langle 1 | \hat{t} + \hat{u} | 1 \rangle = \frac{5}{4} \hbar \omega \left(x^2 + \frac{1}{x^2} \right) \quad (6)$$

where $x \equiv b/a_{\text{osc}}$, and $a_{\text{osc}}^2 = \hbar/m\omega$. Since ψ_0 and ψ_1 are real and of opposite parity, the only non-zero two-particle matrix elements are

$$V_{0000} = -|U_0| \quad (7)$$

$$V_{1111} = -\frac{3}{4}|U_0| \quad (8)$$

$$V_{0011} = -\frac{1}{2}|U_0| = V_{0101} = V_{0110} = V_{1001} = V_{1100} \quad (9)$$

where

$$|U_0| = \hbar\omega \sqrt{\frac{2}{\pi}} \frac{|a|}{a_{\text{osc}}} \frac{1}{x^3}. \quad (10)$$

By defining $2\epsilon \equiv \hbar\omega(x^2 + 1/x^2)$, we obtain

$$\begin{aligned} \hat{H} = & \frac{1}{2}\epsilon(\hat{a}_1^\dagger\hat{a}_1 - \hat{a}_0^\dagger\hat{a}_0) + 2\epsilon(\hat{a}_0^\dagger\hat{a}_0 + \hat{a}_1^\dagger\hat{a}_1) \\ & - \frac{1}{2}|U_0|\hat{a}_0^\dagger\hat{a}_0^\dagger\hat{a}_0\hat{a}_0 - \frac{3}{8}|U_0|\hat{a}_1^\dagger\hat{a}_1^\dagger\hat{a}_1\hat{a}_1 \\ & - \frac{1}{4}|U_0|(\hat{a}_0^\dagger\hat{a}_0^\dagger\hat{a}_1\hat{a}_1 + \hat{a}_1^\dagger\hat{a}_1^\dagger\hat{a}_0\hat{a}_0) \\ & - \frac{1}{2}|U_0|(\hat{a}_0^\dagger\hat{a}_1^\dagger\hat{a}_1\hat{a}_0 + \hat{a}_1^\dagger\hat{a}_0^\dagger\hat{a}_0\hat{a}_1), \end{aligned} \quad (11)$$

which is of the same form as the Hamiltonian for the Lipkin model [9]. Introducing the so-called quasi-spin operators

$$\hat{J}_z = \frac{1}{2}(\hat{a}_1^\dagger\hat{a}_1 - \hat{a}_0^\dagger\hat{a}_0) \quad (12)$$

$$\hat{J}_+ = \hat{a}_1^\dagger\hat{a}_0, \quad (13)$$

and

$$\hat{J}_- = \hat{a}_0^\dagger\hat{a}_1, \quad (14)$$

which obey the $SU(2)$ algebra of ordinary spin, that is $[\hat{J}_+, \hat{J}_-] = 2\hat{J}_z$ and $[\hat{J}_z, \hat{J}_\pm] = \pm\hat{J}_\pm$, the Hamiltonian can be written as

$$\begin{aligned} \hat{H} = & \epsilon\hat{J}_z + 2\epsilon\hat{N} - \frac{1}{2}|U_0| \left[\frac{\hat{N}}{2} \left(\frac{\hat{N}}{2} - 1 \right) - (\hat{N} - 1)\hat{J}_z + \hat{J}_z^2 \right] \\ & - \frac{3}{8}|U_0| \left[\frac{\hat{N}}{2} \left(\frac{\hat{N}}{2} - 1 \right) + (\hat{N} - 1)\hat{J}_z + \hat{J}_z^2 \right] \\ & - \frac{1}{4}|U_0| (\hat{J}_+ \hat{J}_+ + \hat{J}_- \hat{J}_-) \\ & - \frac{1}{2}|U_0| (\hat{J}_+ \hat{J}_- + \hat{J}_- \hat{J}_+ - \hat{N}) \end{aligned} \quad (15)$$

where $\hat{N} = \hat{a}_0^\dagger\hat{a}_0 + \hat{a}_1^\dagger\hat{a}_1$ is the particle number operator. The dimensionless parameter in the problem is seen to be $N|U_0|/\epsilon$. Furthermore, we introduce the ‘‘Cartesian’’ components of the quasi-spin through $\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y$ and rewrite \hat{H} as

$$\begin{aligned} \hat{H} = & \epsilon\hat{J}_z + 2\epsilon\hat{N} - \frac{1}{2}|U_0| \left[\frac{\hat{N}}{2} \left(\frac{\hat{N}}{2} - 1 \right) - (\hat{N} - 1)\hat{J}_z + \hat{J}_z^2 \right] \\ & - \frac{3}{8}|U_0| \left[\frac{\hat{N}}{2} \left(\frac{\hat{N}}{2} - 1 \right) + (\hat{N} - 1)\hat{J}_z + \hat{J}_z^2 \right] \\ & - \frac{1}{2}|U_0|(\hat{J}_x^2 - \hat{J}_y^2) - |U_0| \left(\hat{J}_x^2 + \hat{J}_y^2 - \frac{\hat{N}}{2} \right). \end{aligned} \quad (16)$$

Since the total spin $\hat{J}^2 = (\hat{J}_+ \hat{J}_- + \hat{J}_- \hat{J}_+)/2 + \hat{J}_z^2$ commutes with \hat{H} , the eigenstates and eigenvalues can be obtained exactly by diagonalizing $(2J+1) \times (2J+1)$ matrices. For N particles, the ground state is found among configurations having $J = N/2$. We can also solve the problem analytically in the semi-classical approximation. In this approach the angular momentum operators become c-numbers and we take

$$J_x = \frac{N}{2} \sin \theta \cos \phi, \quad (17)$$

$$J_y = \frac{N}{2} \sin \theta \sin \phi, \quad (18)$$

and

$$J_z = \frac{N}{2} \cos \theta. \quad (19)$$

Upon substituting these expressions in \hat{H} , and taking $N/2(N/2 - 1) \approx N^2/4$, $N - 1 \approx N$, we find the semi-classical expression for the energy of the system

$$\begin{aligned} E = & \frac{N\epsilon}{2} \cos \theta + 2\epsilon N - \frac{1}{2}|U_0| \left[\frac{7N^2}{16} - N \right. \\ & \left. - \frac{N^2}{8} \cos \theta + \frac{7N^2}{16} \cos^2 \theta + \frac{N^2}{4} \sin^2 \theta (2 + \cos 2\phi) \right]. \end{aligned} \quad (20)$$

This quantity is for fixed θ clearly minimized by $\phi = 0$, and thus the energy per particle can be written as

$$\begin{aligned} \frac{E}{N} = & \frac{1}{2} \left(\epsilon + \frac{N|U_0|}{8} \right) \eta + \frac{5N|U_0|}{32} \eta^2 \\ & - \frac{1}{2} \left(\frac{19N}{16} - 1 \right) |U_0| + 2\epsilon \end{aligned} \quad (21)$$

with $\eta \equiv \cos \theta$. Equilibrium occurs at the value η_0 of η given by

$$\eta_0 = \begin{cases} -1, & \frac{N|U_0|}{\epsilon} < 2, \\ -\left(\frac{1}{5} + \frac{8\epsilon}{5N|U_0|}\right), & \frac{N|U_0|}{\epsilon} \geq 2, \end{cases} \quad (22)$$

and the equilibrium energy is found to be

$$\frac{E_0}{N} = \begin{cases} -\frac{1}{2}[-3\epsilon + (N-1)|U_0|], & \frac{N|U_0|}{\epsilon} < 2, \\ -\frac{1}{10}[-19\epsilon + \frac{4\epsilon^2}{N|U_0|} + (6N-5)|U_0|], & \frac{N|U_0|}{\epsilon} \geq 2. \end{cases} \quad (23)$$

For the population of the lowest single-particle state ψ_0 we get

$$\frac{N_0}{N} = \begin{cases} 1, & \frac{N|U_0|}{\epsilon} \leq 2, \\ \frac{3}{5} + \frac{4\epsilon}{5N|U_0|}, & \frac{N|U_0|}{\epsilon} > 2, \end{cases} \quad (24)$$

Thus we see that the extent to which the condensate is fragmented is determined by the ratio

$$\frac{N|U_0|}{\epsilon} = \sqrt{\frac{8}{\pi}} \frac{1}{x^5 + x} \frac{N|a|}{a_{\text{osc}}}. \quad (25)$$

The quantity $N|a|/a_{\text{osc}}$ will from here on be called the effective coupling. A large effective coupling will give a correspondingly large population of the state ψ_1 . However, since the two-body interaction is attractive the system will collapse if the effective coupling exceeds a critical value. From a variational calculation with only the state ψ_0 taken into account, the critical value is found to be $N|a|/a_{\text{osc}} \approx 0.67$ [10,11], in reasonable agreement with the stability criterion $N|a|/a_{\text{osc}} < 0.58$ obtained by Ruprecht *et al.* from numerical solutions of the time-dependent Gross-Pitaevskii equation [6]. In Fig. 1 we show results for both the exact and the semi-classical calculation of the ground state energy of the Hamiltonian in Eq. (15). The exact solution was obtained numerically. The quantity \hat{H}/N depends on N essentially only through the effective coupling $N|a|/a_{\text{osc}}$, and we checked that it was sufficient to do the calculations with $N = 50$ particles. This made numerical calculations easy, as we simply had to diagonalize 51×51 matrices for various values of the variational parameter $x = b/a_{\text{osc}}$. From Fig. 1 it is seen that the semi-classical solution is very close to the exact one. The critical value of the effective coupling was again found to be ≈ 0.67 . At this low effective coupling, the interaction is not strong enough to excite particles into the state ψ_1 to any appreciable extent, and the result is therefore nearly identical to the calculation of Ref. [11]. This is reflected in the occupation number for ψ_0 , shown as a function of $N|a|/a_{\text{osc}}$ in Fig. 2. For all effective couplings which allow for a metastable Bose condensate, all particles condense in ψ_0 . The depletion reaches $\sim 10\%$ at $N|a|/a_{\text{osc}} \approx 3.5$, and approaches 40% in the limit $N|a|/a_{\text{osc}} \gg 1$. The derivative of the semi-classical result for N_0/N is discontinuous at $N|U_0|/\epsilon = 2$, while from Fig. 2 this is not the case for the exact result. This is due to the finite value of N in the exact calculation, as we checked that the edge at $N|U_0|/\epsilon = 2$ became sharper when we increased N .

Our choice of single-particle wave functions led to specific ratios of the interaction strengths V_{0000} , V_{1111} , and V_{1100} . As one could imagine alternative choices for the wave functions (experimentally one could alter the trapping potential), it is worthwhile to check how a change in these ratios affects our results. We use the same form of the Hamiltonian in Eq. (11), but take

$$V_{0000} = -|U_0|, \quad (26)$$

$$V_{1111} = -\alpha|U_0|, \quad (27)$$

and

$$V_{1100} = -\beta|U_0|. \quad (28)$$

In the semi-classical approximation the energy per particle becomes

$$\begin{aligned} \frac{E}{N} = & \frac{1}{2} \left[\epsilon + \frac{(1-\alpha)N|U_0|}{2} \right] \eta + \frac{N|U_0|}{8} (6\beta - \alpha - 1) \eta^2 \\ & - (2 + 2\alpha + 3\beta) \frac{N|U_0|}{4} + 2\epsilon \end{aligned} \quad (29)$$

neglecting constant terms of order 1 compared with N . Minimizing with respect to η we find that the population of the lowest single-particle state is given by

$$\frac{N_0}{N} = \frac{3\beta - \alpha}{6\beta - \alpha - 1} + \frac{\beta}{6\beta - \alpha - 1} \frac{\epsilon}{N|U_0|} \quad (30)$$

and we see that we could get a significant fragmentation of the condensate even with $N|U_0|/\epsilon \sim 1$ if we could make β large. However, the elementary inequality

$$\int d^3r |\psi_0|^4 + \int d^3r |\psi_1|^4 \geq 2 \int d^3r |\psi_0|^2 |\psi_1|^2, \quad (31)$$

which gives $1 + \alpha \geq 2\beta$, will in practical situations prohibit us from designing the two-body matrix elements so that significant fragmentation is obtained. If $1 + \alpha = 2\beta$ then $|\psi_0|^2 = |\psi_1|^2$, i.e. ψ_0 and ψ_1 are identical and there is no fragmentation.

To conclude, we have examined a simple two-level model to see whether an attractive interaction favors the formation of a fragmented Bose-Einstein condensate. Our results indicate that the answer to this question is no: at the coupling strengths where a metastable state exists, all particles condense in the state ψ_0 . We have only considered the case of condensation in an isotropic harmonic oscillator potential, and the situation could be different if one were free to design the relative strengths of the two-body matrix elements involved in the calculation. However, the inequality (31) must be satisfied, and this seems to prevent us from choosing the strengths so that fragmentation is obtained. Thus the conclusion remains the same as in the homogeneous case considered by Nozières and St. James [8]: the system will collapse before a fragmented Bose condensate can form. We remark that our results are consistent with those of Wilkin *et al.* [12], who found no fragmentation for bosons with weakly attractive interactions in the absence of rotation.

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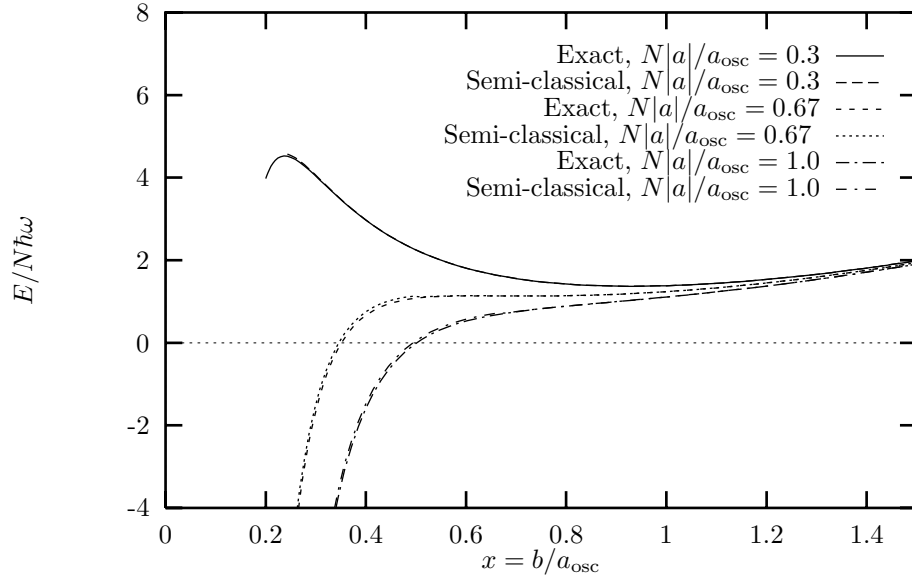


FIG. 1. Comparison of the exact and semi-classical result for the energy per particle.

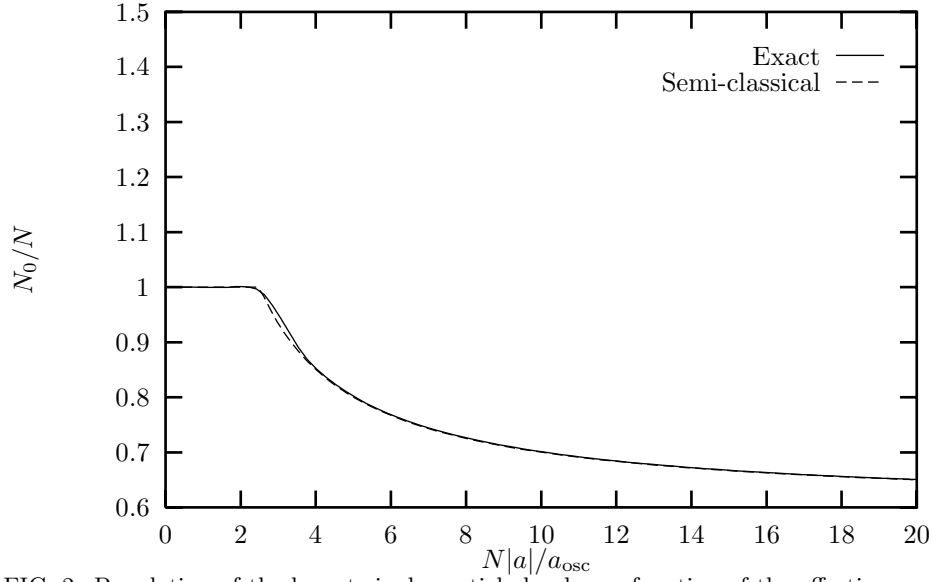


FIG. 2. Population of the lowest single-particle level as a function of the effective coupling. The exact result is for $N = 50$ particles.